Substituent Effects on the Aromaticity of Cyclopropenium Analogues

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The cyclopropenyl ion and several of its derivatives have attracted the interest of experimental and theoretical chemists [1-3]. Aromaticity is of fundamental importance to chemistry [4]. Herein, we wish to report the structures, energies, and aromaticities of unsaturated three-membered rings with the help of the Gaussian 09 program using the B3LYP theory and the 6-311+G(d,p) basis set. Aromatic stabilization energies (ASE) were also evaluated from nucleus-independent chemical shift (NICS) values of title molecules. All of the studied compounds obey the rule of Hückel $(4n+2)\pi$ electron species. However, the inclusion of Si and Ge elements heavier than carbon decreases the aromaticity.

To what extent are the aromaticities of these three membered rings affected by their substituents? For this question, the effect of substitution of cyclic system can be quantitatively examined by sEDA and pEDA parameters. The calculated sEDA and pEDA descriptors correlated with NICS and ASE values.

X: Si and Ge
Y: -BeH, $-BF_2$, $-BH_2$, -Br, $-CF_3$, $-CH_3$, -Cl, -CN,
- F, -H, -Li, $-NH_2$, $-NO_2$, $-OCH_3$, -OH, -Ph,
$-SCH_3$, -SH, $-SiH_3$, $SiMe_3$, -*t*-Butyl.

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